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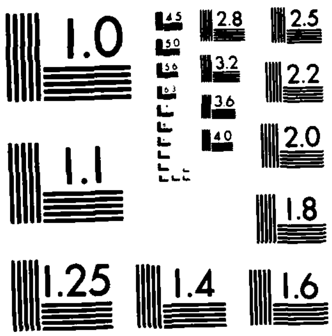

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Physical mathematics
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This work on this project dealt with large scale scientific computing. Particular attention was given to fluid flow - both compressible and incompressible - chemically reacting flows arising in combustion as well as moving boundary problems. The primary object was to develop efficient numerical methods that could be used for practical engineering problems. The research consisted in the development of appropriate variational formulations, and then inventing stable and accurate discretizations based on the variational methods. - continued on reverse.

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20. Abstract continued.

In the area of combustion this has lead to an entirely new approach which has proven effective in modelling the very complicated features of chemically reacting flows.

NUMERICAL METHODS FOR FREE BOUNDARY PROBLEMS AND TWO PHASE FLOWS

FINAL REPORT

George J. Fix

July 19, 1983

U. S. ARMY RESEARCH OFFICE

Contract DAAG29-80-C-0081

Carnegie-Mellon University

DAAG29-80-C-0081 George J. Fix

1 March 1980 - 28 February 1983

The work supported by this contract centered around the following problem areas:

1. Finite Element Methods for flow problems
2. Numerical methods for free boundary problems
3. Finite difference methods for chemically reacting flows

Work on the first problem

The work on flow problems using finite element techniques is contained in references [1], [5], [7], [9], [10], [12], and [13].

The techniques offer many advantages for modelling practical flow problems. They are well suited to complicated geometries and irregular grids that can be used without difficulty. They do, however, have one major drawback. Many of the finite element spaces which have been successfully used in elliptic problems have serious instabilities when applied to flow problems. Because of this, a good deal of attention has been given to developing criteria for determining when a particular element will be stable, and then using this to invent new stable elements that can be conveniently used in practical problems. This is the main thrust in papers [1], [5], [7], [10], and [13].

Compressible flows offer far more difficulties than incompressible flows. Indeed, as in shown in [9] there are many elements which are stable in the incompressible case yet unstable in the compressible case. It was shown in [9] that the key is mass conservation, and a number of new mass conserving elements were introduced which are stable for compressible flows.

Research on numerical methods for compressible flows has also dealt with different types of variational principles, and in particular schemes of the least square type. This is discussed in [9], while in [12] it is applied to a transonic flow problem.

Work on the second problem

Research has centered here on a new model for free boundary problems where the phase ϕ of the material is a part of the model to be computed along with the temperature field T. Introducing a Helmholtz free energy functional, a nonlinear system of parabolic partial differential equations can be developed for ϕ and T. This has been called a phase field model of free boundary problems. This system involved two parameters ξ (a diffusion length for ϕ) and τ (a relaxation time), and using singular perturbation expansions one can show that the phase field model is correct as ξ, τ suitably approach 0. In [8] this model was applied to a number of Stefan type problems as well as problems having effects due to supercooling.

Work on the third problem

One of the difficult problems in modelling combustion processes with continuum mechanical models, i.e., partial differential equations, is that some of the variables may become multivalued. This occurs when the paths of two or more particles coincide. In single phase fluid mechanics this is usually when a shock appears, and the governing partial differential equations are replaced with appropriate jump conditions.

In multiphase reacting flow shocks in this sense are not present, and the continuum variables are simply multivalued.

We treated this type of flow with a new Lagrangian based finite difference scheme. This was developed in [6] and successfully applied to selected combustion problems in [2] and [3].

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PARTICIPATING SCIENTIFIC PERSONNEL

1. Tsu-Fen Chen - Graduate Student
   M.S. December 9, 1980
   Ph.D. August 1983

2. Eduardo Socolovsky - Graduate Student
   M.S. March 16, 1982
   Ph.D. Expected June 1984

3. Manil Suri - Graduate Student
   M.S. September 1, 1981
   Ph.D. August 1983

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